

		PnpA
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<u>Data Collection</u>		
	Space Group	P2 ₁ 2 ₁ 2 ₁
	Wavelength (Å)	0.9786
<i>Cell dimensions</i>		
	a,b,c (Å)	76.6, 110.0, 130.9
	Resolution (Å)	38.3 - 1.40 (1.45 - 1.40)
	Number of observations measured	1,194,493 (115,963)
	Number of unique reflections measured	216,685 (21,426)
	Multiplicity	5.5 (5.4)
	Completeness (%)	99.8 (99.4)
	I/σ	18.9 (0.85)
	Wilson B-factor	20
	R _{merge}	0.046 (1.47)
	CC (1/2) (%)	100 (61.6)
	Monomers per asymmetric unit	2
	Matthews coefficient (Å ³ Da ⁻¹)	2.45
	Solvent content (%)	49.9
<u>Refinement</u>		
	R _{work} /R _{free} (%)	14.7 / 17.5
	Numbers of non-hydrogen atoms	8870
	macromolecules	7646
	ligands	169
	water	1055
	Protein residues	914
<i>RMSD from standard stereochemistry</i>		
	Bond lengths (Å)	0.011
	Bond angles (°)	1.08
<i>Ramachandran plot statistics</i>		
	Favored (%)	98.5
	Allowed (%)	1.4
	Disallowed (%)	0.1
PDB Code		6SQX